

PERSPECTIVES ON EXCELLENCE IN MISSION-FOCUSED SCIENCE, TECHNOLOGY, AND ENGINEERING AT LOS ALAMOS NATIONAL LABORATORY // WINTER 2019

Probing the critical role water plays in the properties of molecular compounds

Elevating achievement teamwork, leadership, and success at first-ever A.T.L.A.S. Day

Contributing to science education in our community



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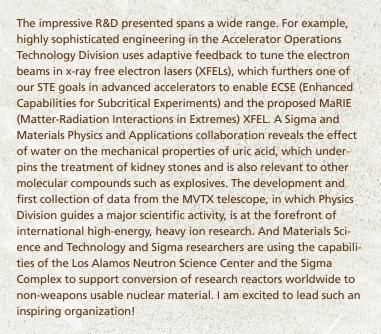
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FROM TONI'S DESK

Toni Taylor, Associate Laboratory Director for Physical Sciences

I am pleased to introduce the first of many *Physical Sciences Vistas*, quarterly reports that will highlight the impressive accomplishments of the personnel in our directorate. This first issue focuses on "excellence in mission-focused science, technology, and engineering" (STE) within Physical Sciences (ALDPS) and includes elements from the three other areas of simultaneous excellence as described in the Laboratory's Agenda.

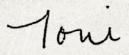


Because the excellence in science and technology so fundamental to our work at the Laboratory is strongly coupled to operational excellence, the continued cultivation of a safe and healthy culture within ALDPS and Los Alamos is an imperative to which myself and Lab leadership are wholly committed. For that reason, I am co-sponsoring, along with Bret Simpkins, associate laboratory director for Facilities and Operations, LANL's LOSA and SAFE activities. LOSA (for Laboratory Operations Supervisors Academy) and SAFE (the Safety Academy for Excellence) comprise intensive, interactive workshops for first-line managers and emerging leaders working with peers across the DOE complex. The ultimate goal is to shape an even stronger-performing, community-based, inclusive working culture across LANL. SAFE and LOSA are founded on the eight Safe Conduct of Research principles that align our cultural expectations. These principles and the associated behavior, listed at right, form the foundation for a strong, high-performing scientific workforce.

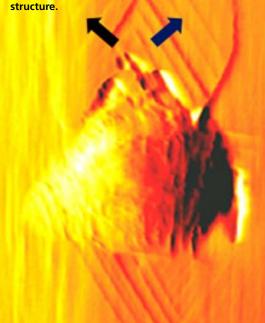
In closing, as we start 2019, I am eager to see what discoveries and accomplishments lie ahead and look forward to learning more about ALDPS and the impressive personnel that make this organization such an essential part of the LANL mission.

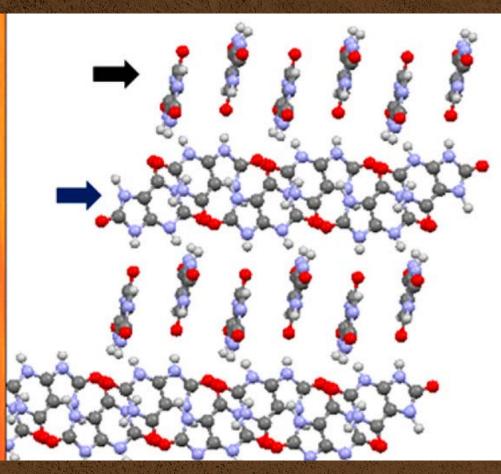
Principles of Safe Conduct of Research

- Everyone is personally responsible for ensuring safe operations.
- Leaders value the safety legacy they create in their discipline.
- Staff raise safety concerns because trust permeates the organization.
- Cutting-edge science requires cuttingedge safety.
- A questioning attitude is cultivated.
- · Learning never stops.
- Hazards are identified and evaluated for every task, every time.
- A healthy respect is maintained for what can go wrong.



Nanoscale mechanical indents in uric acid produce defined steps visible in post-indent images, which are crystallographic slip steps perpendicular to hydrogen bonding ribbons in the crystal structure. The arrows denote directions perpendicular to the slip steps and the associated hydrogen bonding ribbons in the structure.





Uric acid crystal study reveals water's effect on mechanical properties of molecular compounds

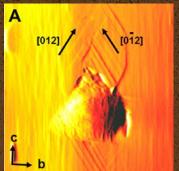
Could help refine treatment for kidney stones; leverages Lab's mission-focused STE expertise

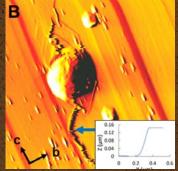
A large percentage of molecular compounds—materials ranging from explosives to pharmaceuticals—can crystallize in different hydration states. This makes understanding how water affects their physical properties—such as solubility, thermal stability, and hardness—a critical research focus.

The uric acid crystals that make up kidney stones can exist in both hydrated and anhydrous (water-free) forms. Both forms share a similar two-dimensional layer structure, making uric acid a particularly useful crystal system for examining the contribution of water molecules to overall mechanical properties.

A team of researchers from Georgetown University, Finishing Manufacturing Science (Sigma-2), and the Center for Integrated Nanotechnologies (MPA-CINT) used nanoindentation and atomic force microscopy (AFM) to assess how these two crystal forms responded to localized surface stresses.

Their results, which showed that anhydrous uric acid is substantially harder and more brittle than hydrated uric acid, are valuable for understanding fundamental materials science and as a base-





Post-indent images of anhydrous uric acid (100) resulting from cono-spherical indents at loads of (A) 2000 micronewtons and (B) 5000 micronewtons. Whereas hydrated stones showed nondescript deformation and creep, these anhydrous stones display distinct "steps" that correlate with discrete crystallographic deformation, labeled with three-number crystal direction indices in (A) and at higher loads as in (B), distinct fracture behavior with much higher step heights, as shown in the plot.

line for understanding the formation and treatment of kidney stones, according to Sigma scientist and co-author Dan Hooks. The journal Chemistry of Materials published the work.

Their post-indent imaging revealed slip planes in preferred crystallographic directions and oriented crack formation at higher peak indentation loads. By contrast, the hydrated forms were much softer and had substantial creep in response to indentation. From time-lapsed images of hydrated crystal indents, the researchers found that some amount of "self-healing" on the surface may be possible at shallow indentation depths of ~100 nm.

"Mechanical perturbation is one current method of treating kidney stones," Hooks said. "Real stones are a mixture of hydrated and anhydrous forms, with a large amount of impurities. Determining and controlling the mechanical properties of these labgrown pure stones in both forms is a first step that could eventually help develop better treatments. In ongoing work, we are investigating the effects of impurities as a model for real stones."

The study relied on Los Alamos National Laboratory's expertise in AFM and nanoindentation, which involve indentation hardness tests applied to small volumes of materials. These localized test methods are ideal for testing relatively fragile, brittle materials, which include pharmaceutical materials, biological materials, and even explosives. It is this unlikely link that has enabled this study, as the LANL team has spent more than 10 years developing the intricacies of the technique to apply to materials of this kind; the team previously delivered some of the first conclusive results for certain types of explosive materials.

Mission connection: The work supports the Laboratory's Nuclear Deterrence and Global Security mission areas and its Materials for the Future science pillar by expanding understanding of defects and interfaces and improving controlled functionality, which is central to the Laboratory's materials strategy.

Reference: "Mechanical properties of anhydrous and hydrated uric acid crystals," Chemistry of Materials, 30 (2018).

Researchers: Fan Liu (Georgetown University); Daniel E. Hooks (Finishing Manufacturing Science, Sigma-2); Nan Li and Nathan A. Mara (Center for Integrated Nanotechnologies, MPA-CINT); and Jennifer A. Swift (Georgetown University). Jennifer Martinez and Lisa Phipps (MPA-CINT) contributed to crystal growth efforts.

Funding: Work was funded by the National Science Foundation and performed in part at CINT, a DOE Office of Basic Energy Sciences user facility jointly operated by Sandia National Laboratories and Los Alamos National Laboratory.

Technical contact: Daniel Hooks

scientist, Neutron Science and Technology esearch



Mandie Gehring specializes in perfecting instrumentation and assessing data for radiography experiments performed at the Lab and elsewhere, Pulsed radiography uses x-ray bursts to image dynamic motion. Using radiography Gehring tests materials that are often key to qualifying the nation's nuclear stockpile.

She leads P-23's National Security Science team and is the principal investigator of radiography for the future Red Sage series, which is being led by Los Alamos researchers to better measure ejecta from plutonium. She is the recipient of two NNSA Defense Programs Awards of Excellence and is part of a Laboratory Directed Research and Development (LDRD) project pairing experiments with simulation to develop a material for more resilient radiation detectors.

"The different problems the stockpile faces in the future will require far more projects like this one, which integrates models with traditional experiments," Gehring said of the LDRD project. "I'm very excited to return to a chemistry lab, and I hope to contribute to the development of synthesis methods for these new, inorganic materials."

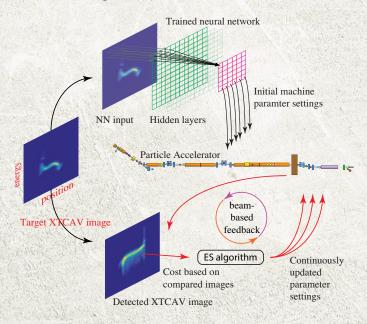
The resulting capability will benefit global security, the medical imaging field, and Enhanced Capabilities for Subcritical Experiments, which is the next major radiographic facility planned in the United States.

Automatically tuning electron beams in advanced XFELS

Next-generation particle accelerators, such as the Linac Coherent Light Source (LCLS) at the SLAC National Accelerator and future instruments such as the proposed MaRIE (Matter-Radiation Interactions at Extremes) x-ray free-electron laser (XFEL) at Los Alamos, support NNSA missions. Due to the complexity and uncertainty inherent in their beam generation, quickly and precisely tuning the sophisticated parameters required to accommodate various experimental setups is challenging. This causes valuable beam time lost between setups.

To mitigate this, a team led by Alexander Scheinker (Radio Frequency Engineering, AOT-RFE) with collaborators from SLAC National Accelerator Laboratory is developing a novel hybrid tuning technique to combine machine learning and adaptive feedback to enable fast, automated optical tuning of the particle beams and optimized beam maintenance over time. The team combined a neural network with adaptive feedback to achieve performance beyond what either method could reach on its own.

The team demonstrated proof-of-principle of this technique at the LCLS, training a neural network to map two-dimensional (2D) longitudinal phase-space distributions of the electron beam. The neural network quickly searched for the desired phase space distribution and then used feedback to determine the correct settings for two different parameters. This network also tracked the correct settings as the accelerator varied over time.



An illustration of the neural network that provided proof-of-principle for the technique. This network was designed to map two-dimensional longitudinal phase space distributions of the LCLS electron beam to LCLS parameter settings. Acronyms: XTCAV = x-band radio frequency transverse deflecting cavity, NN = neural network, ES = extremum seeking.

For this initial study, the team focused on just two parameters of the LCLS, which control how much the electron beam is compressed. The researchers performed a 2D grid scan of the parameters and saved a 2D longitudinal phase space distribution at each point. The investigators used the data to train a neural network to predict parameter settings based on 2D phase space distributions. They created a target phase space distribution (not part of the training data) by making large changes in parameter settings. The team used the neural network to predict what the machine parameter settings should be to achieve this target. Because the network must interpolate between training points and the machine characteristics drift with time, the predicted parameter settings resulted in a distribution close to the target but not an exact match.

The researchers used model-independent feedback, which completed the tuning by zooming in on the actual correct parameter settings and continuously tracking them as they varied with time. In this demonstration, the target phase space was so dramatically different from the initial machine setup that local model-independent feedback alone became trapped in a local minimum, unable to converge to the correct settings. The team intends to create non-invasive diagnostics that account for the 6 dimensions of phase space and plans to apply the algorithm to tune about 20 parameters at once.

The core algorithm will benefit all particle accelerators, including the linear accelerator at the Los Alamos Neutron Science Center. The types being developed would especially benefit the Lab's proposed MaRIE XFEL for exploring matter-radiation interactions in extremes. Because MaRIE would be designed to produce extremely closely spaced electron bunches, it would face greater tuning, control, and optimization challenges than existing accelerators.

Mission connection: The work supports the Laboratory's Nuclear Deterrence mission area and its Nuclear and Particle Futures science pillar, especially its accelerators and electrodynamics thrust area.

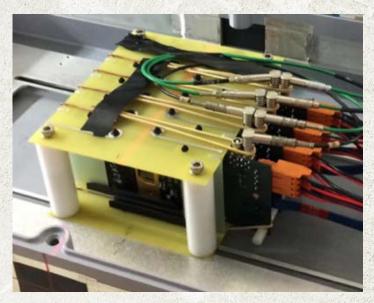
ET THE DETAILS

Reference: "Demonstration of model-independent control of the longitudinal phase space of electron beams in the Linac Coherent Light Source with femtosecond resolution," *Physical Review Letters*, 121 (2018)

Researchers: Alexander Scheinker (Radio Frequency Engineering, AOT-RFE); Auralee Edelen, Dorian Bohler, Claudio Emma, and Alberto Lutman (SLAC National Accelerator Laboratory).

Funding: The Laboratory Directed Research and Development program funded the work at Los Alamos through its 2018 Momentum Initiative, which aimed to advance two capability thrusts: accelerator capability enhancement and development of advanced accelerators and exploration of mesoscale materials phenomena using state-of-the-art light source user facilities. **Technical contact:** Alexander Scheinker

New MVTX telescope collects first data for planned DOE flagship physics experiment



Four MAPS sensors, located inside the telescope box, are stacked in the path of the beam.

Working at Fermi National Accelerator Laboratory, a research team headed by members of Subatomic Physics (P-25) performed the first test of a prototype detector, proving that this state-ofthe-art technology could collect data on high-energy, heavy ion collisions. The team developed the MVTX (for monolithic active pixel sensor [MAPS]-based vertex detector) to better identify origin vertices of particle tracks for sPHENIX, a planned DOE flagship experiment in nuclear physics.

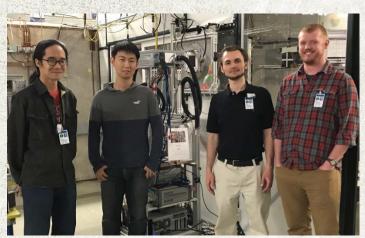
sPHENIX is proposed to study the nature of subatomic particles known as quark gluon plasma (QGP). QGP was the universe's dominant material in the first few microseconds after the Big Bang. Better understanding of it could help explain how the universe was created and improve cosmology research.

Because QGP only exists for short periods and only at extremely high temperatures and densities, it has proven difficult to measure. sPHENIX will address this challenge by providing worldclass, large-scale capabilities for future multi-scale QGP studies. sPHENIX, which is planned for Brookhaven National Laboratory's Relativistic Heavy Ion Collider (RHIC), will use fully reconstructed jets and high-precision upsilon spectroscopy at high beam-collision rates to make unprecedented measurements.

The MVTX adds a key capability to this suite—it can identify jets containing heavy subatomic particles called bottom quarks. A particle tracker with unique vertex resolution and high-rate capability is required to distinguish heavy-flavor jets from the other particles produced in heavy ion collisions. Los Alamos researchers proposed the MVTX as a high-speed, large-acceptance precision vertex detector that would help sPHENIX measure bottom quarks, which in turn are precision diagnostics for the QGP. The effort combines high-level physics and technical capabilities to provide important data inputs for the full sPHENIX program.

The MVTX's development for sPHENIX is only one of many potential uses for MAPS-based technology. Lab staff are exploring the technology for programs such as the one at the future Electron-Ion-Collider facility at Brookhaven. The technology may also have applications in the high-precision imaging work proposed as part of the Dynamic Mesoscale Materials Science Capability, the project formerly known as MaRIE.

Mission connection: The work supports the Lab's Fundamental Science mission and the Nuclear and Particle Futures science pillar by developing expertise and capabilities required for national security science missions. Through MVTX's development, the Lab leads a major scientific activity at the forefront of international high-energy, heavy ion research.



Los Alamos researchers (from left) Sho Uemura, Sanghoon Lim, Alex Tkatchev, and Darren McGlinchey in front of the MVTX telescope at Fermilab.

Researchers: Hubert van Hecke, Chris O'Shaughnessy, Walt Sondheim, Alex Tkatchev, Sho Uemura, Sanghoon Lim, Darren McGlinchey, Xuan Li, Pat McGaughey, Kun Liu, Cesar da Silva, Andi Klein, Alex Wickes, and Ming Liu (all Subatomic Physics, P-25); Mark Prokop (Radio Frequency Engineering, AOT-RFE); Ivan Vitev, Chris Lee, Rajan Gupta, Zhongbo Kang, Haitao Li, and Varun Vaidya (Nuclear and Particle Physics, Astrophysics, and Cosmology, T-2); Jerome Olivier Daligault (Applied Mathematics and Plasma Physics, T-5); and Boram Yoon (Applied Computer Science, CCS-7).

Funding: The Laboratory Directed Research and Development program funds the prototype detector's development.

Technical contact: Ming Liu

OPERATIONAL EXCELLENCE

A.T.L.A.S. Day = teamwork, leadership, success



Joe Dabney (LANSCE Facility Operations, LANSCE-FO) kicks off A.T.L.A.S Day.

"These testimonials delivered the message of how a 'life-changing event'—a single accident—can impact not only the individual worker but the families and communities where this individual worked and lived. What a powerful message!"

"I learned a ton and appreciated the opportunity to network as well. The variety of topics, interests, and the organization of the day were very good."

"The presentations and workshops offered in the afternoon made me realize how far the WSSTs have come in truly engaging and involving the workforce in concert with management on defining true, measurable, and realistic achievement goals for improving the safety and security culture at LANL."



Self-defense demonstration by Gracie Barra Jiu-Jitsu.



Reanna Cline (PIO-Construction Management, PIO-CM) facilitates a seminar on personal experiences.

While being mindful of safety can seem mundane, the Lab's first-ever A.T.L.A.S. Day was anything but. A.T.L.A.S. (for achieving teamwork, leadership, and success) drew more than 170 employees to the Los Alamos Neutron Science Center (LANSCE) for a day that included live music, personal testimonials, self-defense lessons, and instruction on falling—safely.

The event began with presentations by Bob Brennecke (LANSCE Facility Operations, DESH-LFO) on improving safety culture with the Voluntary Protection Program and by Stanley Trujillo (Performance Assurance, IQPA-PA) on operating experience at the Laboratory.

Participants could choose from a variety of workshops that included:

- Stress and conflict management
- · Security at home
- Workplace violence prevention
- Self defense
- Cybersecurity
- Diversity awareness

Special events included a health fair, a panel discussion by the Lab management team, a pizza lunch, giveaways and drawings, and an acoustic music performance by Lab employee and country musician Sim Balkey (PPS Project Controls, PPS-PC).

The event was sponsored by the Lab's Worker Safety and Security Teams (WSSTs), the Associate Directorate for Project Management (ADPM), the Associate Directorate for Mission Assurance, Security, and Emergency Response (ADMASER), the Associate Directorate for Environment, Safety and Health (ADESH), LANSCE, and the LANL Operating Experience Program (OPEX).



The team that made A.T.L.A.S Day a reality.



Deputy Director of Operations Kelly Beierschmitt (left) meets with an A.T.L.A.S. Day attendee.

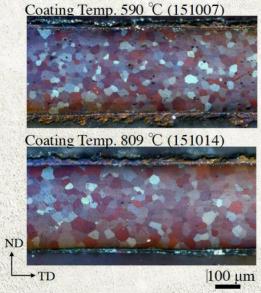
ToF neutron diffraction reveals texture changes in low-enriched metallic uranium nuclear fuel

Advances efforts to reduce amounts of highly enriched uranium

The United States is committed to further strengthening nuclear security and nonproliferation to reduce the threat of terrorists acquiring nuclear material. To meet this important mission, Los Alamos is bringing its expertise to the task of converting research reactors worldwide to use low-enriched uranium (LEU) fuels—which cannot be used in weapons—rather than highly enriched uranium fuels, for the NNSA's Convert program.

To aid the development of a widely applicable LEU fuel, Laboratory materials scientists examined the microstructural changes that occur during the fuel fabrication process, a relatively unexplored area of study. Their work revealed texture changes during processing—changes that affect the material's properties. Understanding these properties is critical to efficiently and economically manufacturing LEU fuel.

Using the promising high-density U-10 wt% Mo (a uranium-molybdenum alloy clad in 6061 aluminum), the researchers applied a zirconium (Zr) coating that acts as a diffusion barrier between

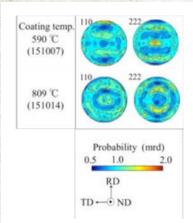


Optical micrographs of two zirconium-coated samples: 151007 and 151014 coated at the lowest and highest temperature, respectively. Both samples showed equiaxed grains, suggesting a recrystallized microstructure, and the grains were coarser near the coating surface than in the center. For the surface regions exposed to plasma spraying, the average grain size for the lowest temperature agreed with the grain size at the center line. Contrarily, the grain size for the sample at the maximum temperature showed an increase of 27.5% relative to the center line grain size.

the fuel and aluminum cladding by means of a Sigma Division-developed plasma-spray technique recognized as a fast and economical coating method. The researchers performed time-of-flight (ToF) neutron diffraction on HIPPO, the high-pressure-preferred orientation instrument at the Los Alamos Neutron Science Center (LANSCE), to reveal the microstructure evolution caused by various plasma temperatures.

Their quantitative texture analysis showed that the texture drastically changed at high coating temperatures, likely due to selective grain growth. This finding agrees with microscopy showing larger grains in these samples closer to the coated surface than in the unaffected center volume. Furthermore, the Zr coating showed a preferential orientation, which could be related to the initial texture of the uncoated U-10Mo. This orientation could be explained by epitaxial growth of Zr on the U-10Mo substrate.

Mission connection: The research supports the Lab's Nonproliferation and Energy Security mission areas and Materials for the Future science pillar. The plasma spray technique leverages the manufacturing science expertise and capabilities of the Laboratory's Sigma Complex, which supports a large, multidisciplinary materials technology base. ToF diffraction used capabilities at LANSCE, which uses intense pulsed protons to produce the wide energy spectrum of spallation neutrons needed to interrogate materials.



(110) and (222) pole figures for gamma U-10Mo for the lowest (590 °C) and highest (809 °C) plasma coating temperatures. The pole figures of the lowest coating temperature are almost identical to the uncoated material, while the pole figures for the sample processed at the highest coating temperature show a clear change of the microstructure.

Reference: "Texture evolution in U-10Mo nuclear fuel foils during plasma spray coating with Zr," Quantum Beam Science 2, 12 (2018).

Researchers: Shigehiro Takajo (Materials Science in Radiation and Dynamics Extremes, MST-8); Kendall J. Hollis and Dustin R. Cummins (Fabrication Manufacturing Science, Sigma-1); Eric L. Tegtmeier (Finishing Manufacturing Science, Sigma-2); David E. Dombrowski (Sigma-1); and Sven C. Vogel (MST-8).

Funding: DOE/NNSA's Office of Material Management and Minimization Reactor Conversion Program (LANL Program Manager Dave Dombrowski).

Technical contact: Sven Vogel

First direct 3D x-ray diffraction imaging of dislocations in polycrystalline metals under tensile loading

Technique aids endeavors in the grand scientific challenge of creating materials by design

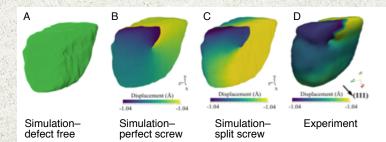
Dislocations accompanying high strain loads in materials are ubiquitous. These defects in a material's structural framework influence a range of materials properties, e.g., from mechanical strength to failure, battery performance, radiation resistance, and crystal growth and dissolution. As a result, researchers have sought to tailor material response through defect engineering and control since these defects were first visualized more than 50 years ago using transmission electron microscopy.

Now, researchers from Los Alamos and Argonne national laboratories have demonstrated a novel advanced imaging technique that offers the promise of accomplishing this more effectively by applying nanometer-scale x-ray strain imaging to materials being pulled apart.

Using Bragg coherent x-ray diffraction imaging at Argonne's Advanced Photon Source (APS), they measured the strain field of a freestanding polycrystalline film after tensile loading. By integrating the observed three-dimensional structure into atomistic modeling, they showed that the measured strain field corresponds to a screw dislocation—that is, a specific form of a dislocation in the crystal's lattice structure.

The work shows the insight enabled by the use of high-energy, advanced light sources, such as the APS and that proposed for NNSA's future Dynamic Mesoscale Materials Science Capability (DMMSC). The mesoscale is the spatial scale where a material's structure and the processing that creates that structure strongly influence its macroscopic behaviors and properties. MaRIE is the Laboratory's proposed facility for studying such dynamic properties at the mesoscale and meeting the mission need for DMMSC. This work also falls under a partner user proposal with researchers Ross Harder and the team at the APS where the joint LANL APS teams are trying to apply these techniques to bulk materials response to damage.

Mission connection: The work supports the Laboratory's Nuclear Deterrence and Global Security mission areas and its Materials for the Future science pillar by advancing efforts aimed at developing materials with controlled functionality and predictable performance, the key objective of the Lab's materials strategy.



Atomic structure and displacement fields with and without a screw dislocation. (A) Atomistic structure obtained by filling copper atoms into the experimentally observed grain. (B) Atomistic structure following addition of a perfect screw dislocation, and (C) atomistic structure after energy minimization. Atoms are colored by their displacement along the (111) from their initial structure. (D) Isosurface rendering of the experimentally imaged copper grain.

T THE DETAILS

Reference: "Three-dimensional x-ray diffraction imaging of dislocations in polycrystalline metals under tensile loading," *Nat. Commun.* 9 (2018). Researchers: Mathew J. Cherukara (Argonne National Laboratory); Reeju Pokharel (Materials Science and Technology, MST-8); Timothy S. O'Leary and J. Kevin Baldwin (Center for Integrated Nanotechnologies, MPA-CINT); Evan Maxey, Wonsuk Cha, Jorg Maser, and Ross J. Harder (Argonne National Laboratory); Saryu J. Fensin (MST-8); and Richard L. Sandberg (MPA-CINT).

Funding: The Los Alamos portion was funded by the Laboratory Directed Research and Development program through its Momentum proposal call, the Dynamic Materials Properties Campaign (C2, LANL Program Manager Dana Dattelbaum) of the Laboratory's Experimental Sciences Program, and the Center for Integrated Nanotechnologies, a DOE Office of Basic Energy Sciences user facility jointly operated by Sandia National Laboratories and Los Alamos National Laboratory.

Technical contact: Richard Sandberg





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